Mesh generation for modeling and simulation of carbon sequestration processes

Mohamed S. Ebeida, Patrick M. Knupp, Vitus J. Leung *
Joseph E. Bishop †, **Mario J. Martinez** ‡

Abstract

Recently, randomly close-packed Voronoi meshes have been proposed for simulating pervasive fracture processes in materials and structures by allowing fractures to grow only at the interelement faces of the polyhedral cells. The polyhedral cells are formulated as finite elements. A new meshing tool is presented here for creating randomly close-packed Voronoi meshes in nonconvex domains with internal surfaces. Applications using these meshes include blast and impact response of engineered structures as well as hydraulic fracturing in geostructures and the design of CO_2 sequestration processes to maintain the integrity of a reservoir caprock that contains pre-existing fractures and joints.

Our meshing approach is based on creating a random cloud of n points whose locations are determined by solving a maximal Poisson-disk sampling problem over nonconvex domains with internal surfaces, required points, and multiple regions in contact. A novel constrained Delaunay algorithm is then utilized to generate Poisson-disk triangulations using $O(n)$ time and memory. The required Voronoi mesh is constructed by retrieving the dual of the triangular mesh. Each phase (sampling, triangulation, Voronoi meshing) of our algorithm utilizes local operations th facilitate parallel implementations. An example of the use of this meshing tool for a fracture simulation is given.

1   Introduction

Under extreme loading conditions most often the extent of material and structural fracture is pervasive in the sense that a multitude of cracks are nucleating, propagating in arbitrary directions, coalescing, and branching. A pure Lagrangian computational method based on randomly close-packed Voronoi tessellations was recently proposed as a robust approach for simulating pervasive fracture processes [1]. In this approach each polyhedral cell is formulated as a finite element, and fractures are allowed to nucleate and grow only at interelement edges in 2D and faces in 3D.

A new meshing tool is presented here for creating randomly close-packed Voronoi meshes in nonconvex domains with internal surfaces. Our fracture meshing algorithm starts with generating a random point cloud by solving a maximal Poisson-disk sampling problem. The associated Constrained Delaunay mesh is then constructed in linear time with respect to the number of points in that cloud. The required random Voronoi mesh then is retrieved as the dual of the Delaunay mesh. The present Voronoi algorithm is limited to domains and fractures that are piecewise linear; however, the domains can be nonconvex. The Voronoi cells have aspect ratios of approximately 1, and the edge and face orientations are unbiased. An analogous 3D Voronoi capability is under development.

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*Computational Sciences and Math, Sandia National Laboratories

†Computational Structural Mechanics, Sandia National Laboratories

‡Thermal & Fluid Processes, Sandia National Laboratories

2 Random Voronoi Meshing

2.1 Poisson-Disk sampling

Poisson-disk sampling is a random process for selecting points from a subdomain of a metric space. A selected point must be *disk-free*, at least a minimum distance, *r*, from any previously selected point. Thus each point has an associated disk of radius *r* that precludes the selection of nearby points. The selected points are called a *sample*, or *distribution*. The sample is *maximal* if no point can be added to it. Euclidean distance is traditional but not essential.

In 2011, we proposed two methods to solve this problem. The first one [2] has a time complexity of $O(n \log n)$ and satisfies the sampling conditions and achieves maximality independent of the round-off error by constructing uncovered areas with geometric primitives. The second method [3] works in any d-dimensional space and has a time complexity of $O(n)$. The performance is improved through the use of a finite sequence of uniform grids with increasing resolutions instead of representing the remaining voids via geometrical primitives. The output of our algorithm is illustrated in Figure 1. A comparison with other sampling methods in Figure 2 shows the efficiency of our approach.
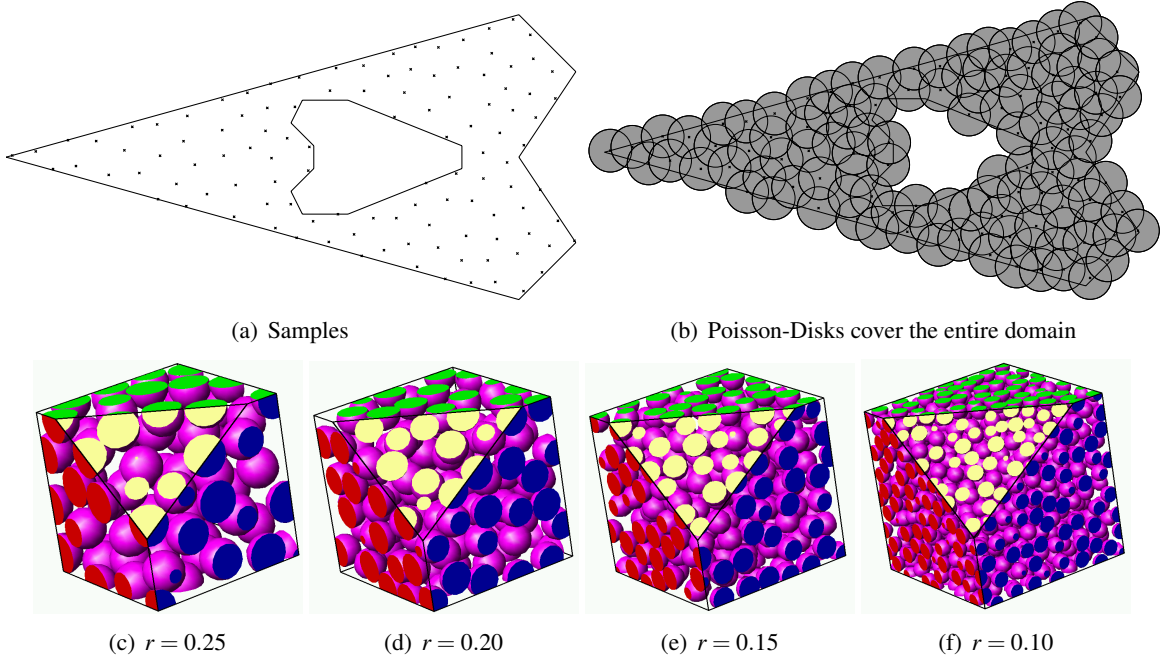

| (a) Samples | (b) Poisson-Disks cover the entire domain |

| (c) $r = 0.25$ | (d) $r = 0.20$ | (e) $r = 0.15$ | (f) $r = 0.10$ |

Figure 1: Poisson-disk sampling of a nonconvex domain (top) and unit cube (bottom). For the 3D case we show nonintersecting sphere with radius $= \frac{r}{2}$.

2.2 Delaunay/Voronoi meshing

The cell structure utilized in our sampling algorithm enables a local, simple, and fast algorithm for constructing the constrained Delaunay triangulation, CDT [4]. This algorithm iterates in constant time over each point p of the maximal Poisson distribution, constructing its star, that is, the triangles containing it. This results in linear total time. Communication between different points is not required except when a nonunique solution exists, that is, more than three points lie on the same circumcircle of one of the generated triangles. The serial implementation was tested on a laptop.[1] The performance

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[1]2010 vintage. Intel® Core™ i7-620M at 2.67 GHz, 4 Mb cache; 4.0 GB RAM; 64-bit Windows 7 OS.
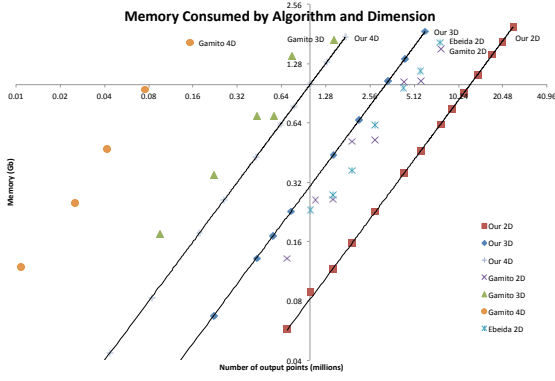
(a) Memory
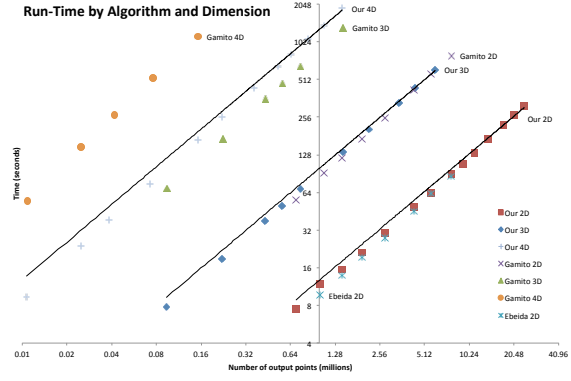
(b) Time

Figure 2: Memory and time used by our sequential MPS implementation vs other sampling codes.

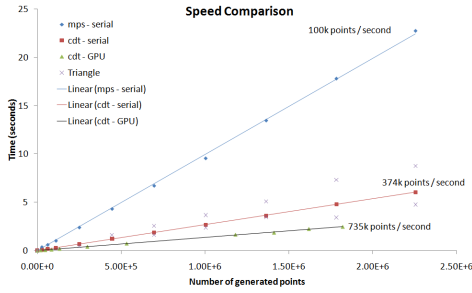and the output of our CDT algorithm illustrate its efficiency in Figure 3 and Figure 4, respectively.

Figure 3: Our serial and GPU CDT implementations show linear performance. Our serial CDT is competitive with Triangle. Our GPU CDT is about a $2\times$ speedup over our serial CDT.
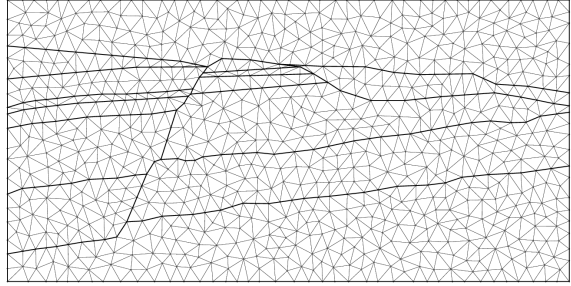

Figure 4: Uniform random CDTs of a seismic domain with internal boundaries. Our implementation was robust even though the user selected a coarser mesh size than the raw boundary allows.

The required random Voronoi mesh is generated by retrieving the dual of the CDT mesh. This operation has to respect the internal and the external boundaries of the domain. Nonconvex Vornoi cells along the boundaries are split into a set of triangles. Moreover, edge collapse operations take place to eliminate all short edges. The capability of our Voronoi meshing tool to handle various domains is illustrated in Figure 5.
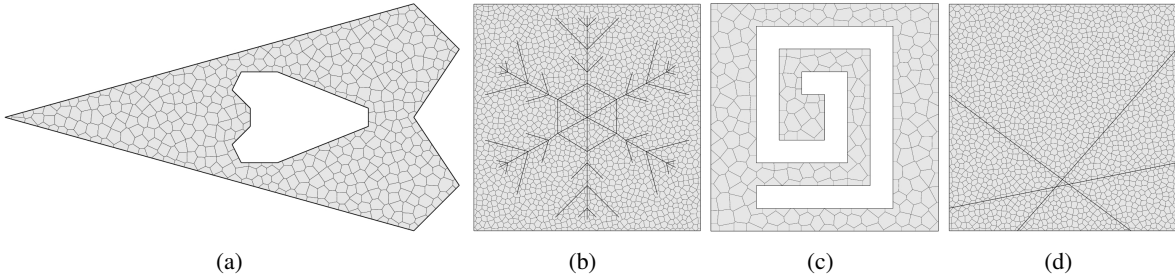

(a)　　　　　(b)　　　　　(c)　　　　　(d)

Figure 5: Our Voroni mesher is capable of handling nonconvex domains with internal boundaries.

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2.3 Hybrid meshing

In 2D, the hybrid mesh capability provides a mechanism for a mesh to have Delaunay, quadrilateral, and Voronoi element types within different subregions of a single domain, as illustrated in Figure 6.

The hybrid mesher sets up the problem for the Delaunay and Voronoi subregions and then calls the algorithms described in the previous subsection. The hybrid capability also contains a simple algebraic method for generating structured quadrilateral meshes on subregionss. The hybrid mesher can be viewed as "glue" between different meshing algorithms; other meshing algorithms could also be included.

The main setup is for the points on the subregion boundaries so that the mesh is conforming. First, the hybrid mesher sets up the problem for the Voronoi subregions with the Delaunay subregions as holes. After the Voronoi subregions are meshed, the hybrid mesher sets up the problems for the Delaunay and quadrilateral subregions with the boundary points added by the Voronoi mesh. Currently, the quadrilateral subregions must be contiguous on the external boundary, and the number of "layers" is an input parameter. Because of the limitations of the Voronoi mesher, the domain and its subregions are limited to piecewise linear geometries.
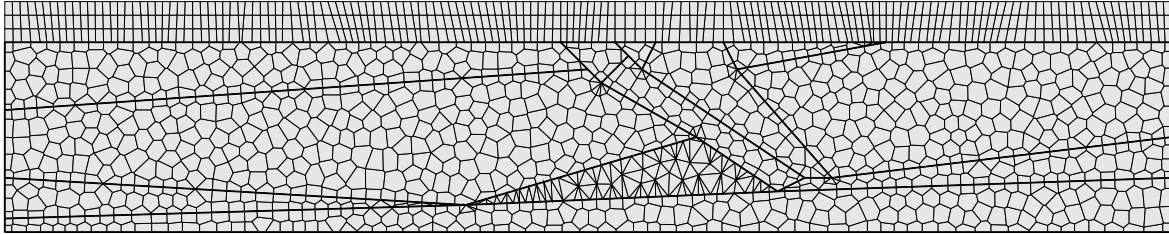

Figure 6: Hybrid mesh.

3 Application Example

In this section we briefly present an application example that uses our meshing tool to create a randomly close-packed Voronoi mesh that conforms to a set of pre-existing geologic fractures shown in Figure 7 in a reservoir caprock layer. The mechanical response and possible growth of these fractures are studied as supercritical CO_2 is injected into the saline acquifer below the caprock, nominally 1000 meters below the surface. The initial fractures represent joints that are initially sealed but are reactivated because of the changing mechanical stress and deformation caused by the injection in the reservoir below the caprock. The nucleation and growth criterion is based on a limit surface of the allowable stress states. A cohesive law is used to model the sealed joints as well as the new fracture surfaces and decays as the cracks open. The Voronoi mesh randomness is viewed as a subset of the inherent material variability (modeled as a random field in the continuum material properties). Thus, this simulation represents one realization of a stochastic process.

4 Conclusions

A new Voronoi and hybrid meshing tool has been created to assist in generating meshes for use in pervasive fracture simulations. The Voronoi mesh capability is based on new algorithms for maximal Possion sampling and constrained Delaunay triangulation. These latter two algorithms constitute significant improvements in previous capabilities and can be applied to other problems outside the context of pervasive fracture modeling. The Voronoi capability has significant speed and memory
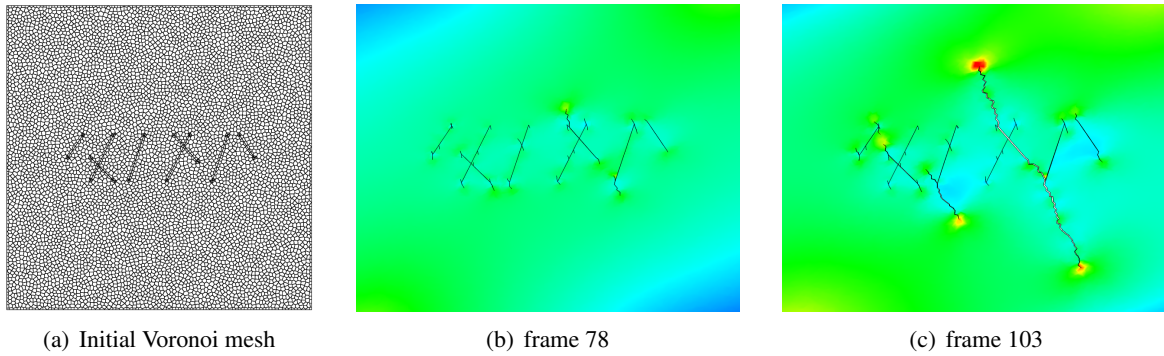
(a) Initial Voronoi mesh   (b) frame 78   (c) frame 103

Figure 7: Mechanical response of a reservoir caprock layer during injection of supercritical CO_2. The color in the pictures represents maximum principal stress. Frames are snapshots of the solution as it progresses in time.

advantages over the capability previously used by the fracture modeling team. Moreover, the domains and fracture networks that can be conformally meshed are notably more complex than those previously available.

The 2D capability has been tested and used in several applications. A 3D capability will soon be delivered. The hybrid capability was developed in a short time by gluing together Voronoi, Delaunay, and algebraic mesh generation algorithms. In the future we hope to extend these capabilities to 3D, with heterogeneously sized elements, and non-piecewise-linear domains.

Acknowledgments

References

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